



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 06:23 PM EDT

PDB ID : 9C5L / pdb_00009c5l
Title : Trypanosoma cruzi beta-3-HBDH R19T/K20S/C64Y mutant in complex with NADH and malonate (C2 space group)
Authors : Hashimoto, H.; Debler, E.W.
Deposited on : 2024-06-06
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

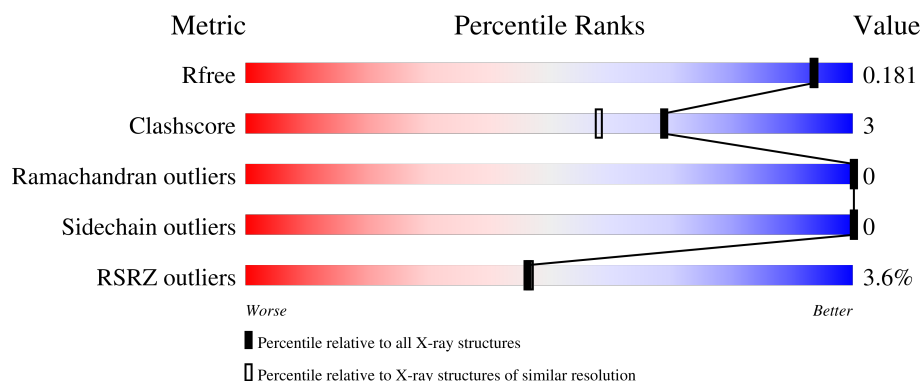
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


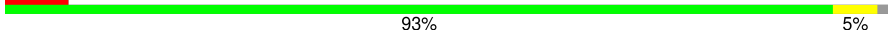


The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	 93%
1	B	270	 93%
1	C	270	 86%
1	D	270	 90%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLI	B	401	-	-	X	-
2	MLI	D	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16655 atoms, of which 7935 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	H	N	O	S	0	5	0
			3936	1231	1982	339	371	13			
1	B	263	Total	C	H	N	O	S	0	2	0
			3935	1233	1982	339	369	12			
1	C	247	Total	C	H	N	O	S	0	5	0
			3734	1171	1888	317	345	13			
1	D	261	Total	C	H	N	O	S	0	2	0
			3896	1221	1961	334	368	12			

There are 28 discrepancies between the modelled and reference sequences:

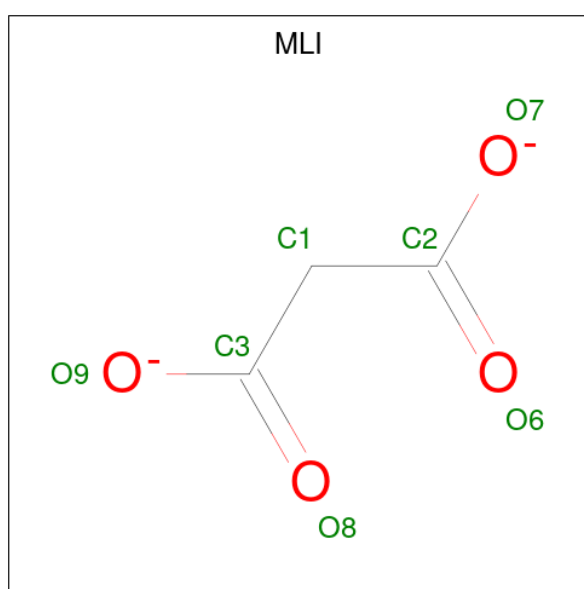
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A2V2VPF1
A	-2	PRO	-	expression tag	UNP A0A2V2VPF1
A	-1	HIS	-	expression tag	UNP A0A2V2VPF1
A	0	MET	-	expression tag	UNP A0A2V2VPF1
A	19	THR	ARG	engineered mutation	UNP A0A2V2VPF1
A	20	SER	LYS	engineered mutation	UNP A0A2V2VPF1
A	64	TYR	CYS	engineered mutation	UNP A0A2V2VPF1
B	-3	GLY	-	expression tag	UNP A0A2V2VPF1
B	-2	PRO	-	expression tag	UNP A0A2V2VPF1
B	-1	HIS	-	expression tag	UNP A0A2V2VPF1
B	0	MET	-	expression tag	UNP A0A2V2VPF1
B	19	THR	ARG	engineered mutation	UNP A0A2V2VPF1
B	20	SER	LYS	engineered mutation	UNP A0A2V2VPF1
B	64	TYR	CYS	engineered mutation	UNP A0A2V2VPF1
C	-3	GLY	-	expression tag	UNP A0A2V2VPF1
C	-2	PRO	-	expression tag	UNP A0A2V2VPF1
C	-1	HIS	-	expression tag	UNP A0A2V2VPF1
C	0	MET	-	expression tag	UNP A0A2V2VPF1
C	19	THR	ARG	engineered mutation	UNP A0A2V2VPF1
C	20	SER	LYS	engineered mutation	UNP A0A2V2VPF1
C	64	TYR	CYS	engineered mutation	UNP A0A2V2VPF1

Continued on next page...

Continued from previous page...

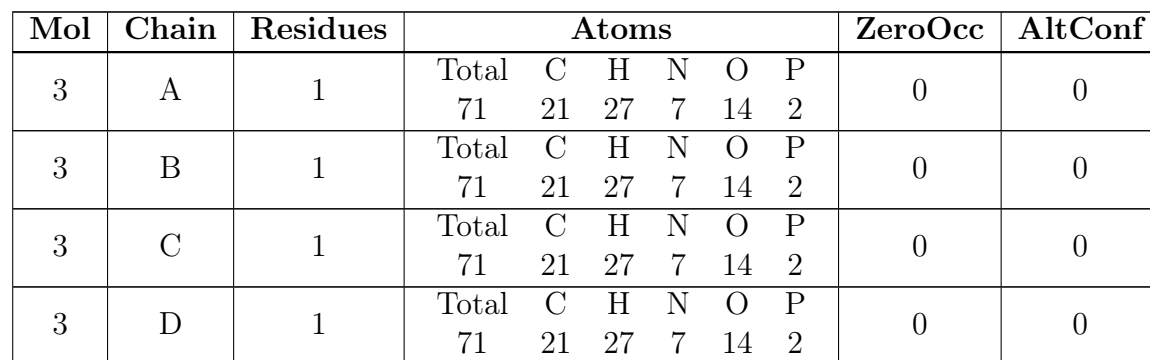
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP A0A2V2VPF1
D	-2	PRO	-	expression tag	UNP A0A2V2VPF1
D	-1	HIS	-	expression tag	UNP A0A2V2VPF1
D	0	MET	-	expression tag	UNP A0A2V2VPF1
D	19	THR	ARG	engineered mutation	UNP A0A2V2VPF1
D	20	SER	LYS	engineered mutation	UNP A0A2V2VPF1
D	64	TYR	CYS	engineered mutation	UNP A0A2V2VPF1

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$) (labeled as "Ligand of Interest" by depositor).

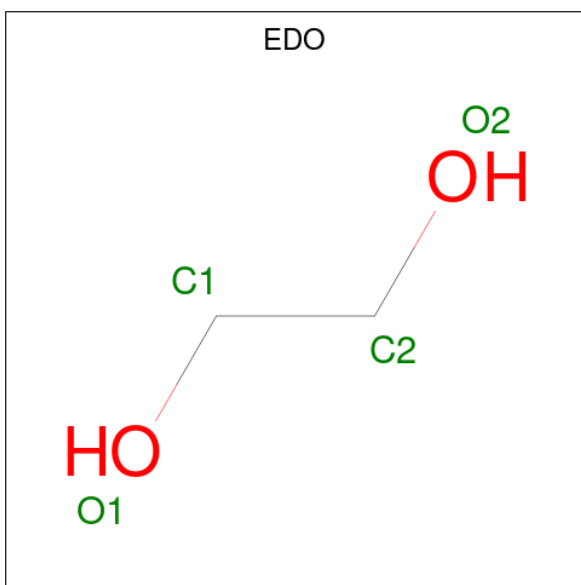


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	2	4		
2	B	1	Total	C	H	O	0	0
			9	3	2	4		
2	C	1	Total	C	H	O	0	0
			9	3	2	4		
2	D	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	246	Total	O	0	0
			246	246		
5	B	199	Total	O	0	0
			199	199		
5	C	213	Total	O	0	0
			213	213		
5	D	166	Total	O	0	0
			166	166		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

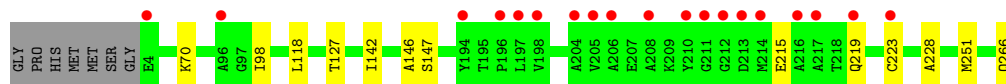
- Molecule 1: Hydroxybutyrate dehydrogenase

Chain A:  93% 5% 2%




- Molecule 1: Hydroxybutyrate dehydrogenase

Chain B:  7% 93% 5%




- Molecule 1: Hydroxybutyrate dehydrogenase

Chain C:  5% 86% 6% 9%



- Molecule 1: Hydroxybutyrate dehydrogenase

Chain D:  2% 90% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.72Å 80.30Å 122.65Å 90.00° 107.58° 90.00°	Depositor
Resolution (Å)	37.97 – 1.60 37.97 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.97-1.60) 99.9 (37.97-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.178 0.158 , 0.181	Depositor DCC
R_{free} test set	2000 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16655	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, NAI, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/2003	0.55	0/2714
1	B	0.39	0/1989	0.49	0/2697
1	C	0.46	0/1889	0.57	0/2563
1	D	0.40	0/1971	0.52	0/2674
All	All	0.42	0/7852	0.53	0/10648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1954	1982	1962	9	0
1	B	1953	1982	1982	12	0
1	C	1846	1888	1888	14	0
1	D	1935	1961	1961	13	0
2	A	7	2	2	0	0
2	B	7	2	2	2	0
2	C	7	2	2	1	0
2	D	7	2	2	2	0
3	A	44	27	27	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	27	27	4	0
3	C	44	27	27	8	0
3	D	44	27	27	4	0
4	D	4	6	6	0	0
5	A	246	0	0	2	0
5	B	199	0	0	3	0
5	C	213	0	0	6	0
5	D	166	0	0	2	0
All	All	8720	7935	7915	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246[B]:SER:OG	5:C:501:HOH:O	1.97	0.81
1:B:215:GLU:OE2	5:B:501:HOH:O	2.01	0.77
1:C:221:PHE:O	5:C:502:HOH:O	2.07	0.73
1:B:266:GLN:O	5:B:502:HOH:O	2.08	0.71
3:C:402:NAI:O2B	5:C:503:HOH:O	2.09	0.70
5:B:502:HOH:O	1:D:266:GLN:O	2.14	0.65
1:A:266:GLN:O	5:A:501:HOH:O	2.15	0.63
1:C:95:ASN:OD1	3:C:402:NAI:H4D	1.99	0.62
1:C:215:GLU:N	5:C:504:HOH:O	2.33	0.61
1:A:251:MET:HE1	1:B:228:ALA:HB3	1.84	0.59
1:D:219:GLN:OE1	5:D:501:HOH:O	2.17	0.57
1:B:146:ALA:O	3:B:402:NAI:H6N	2.05	0.56
1:B:118[B]:LEU:HD21	3:B:402:NAI:N6A	2.20	0.56
1:C:127:THR:HG23	1:C:142[B]:ILE:HD13	1.88	0.56
1:B:219:GLN:NE2	1:B:223:CYS:SG	2.77	0.55
1:A:146:ALA:O	3:A:402:NAI:H6N	2.07	0.54
2:C:401:MLI:C3	3:C:402:NAI:H4N	2.38	0.54
1:D:28:MET:O	1:D:32:MET:HG3	2.08	0.53
1:C:32:MET:HE2	1:C:58:TYR:CE1	2.44	0.53
5:A:501:HOH:O	1:C:266:GLN:O	2.18	0.53
1:D:29:ARG:HH21	1:D:235:GLU:HB3	1.73	0.53
1:C:47:GLU:O	1:C:47:GLU:HG2	2.09	0.53
1:D:29:ARG:NH1	1:D:32:MET:HE1	2.25	0.51
1:D:146:ALA:O	3:D:403:NAI:H6N	2.11	0.50
2:B:401:MLI:C2	3:B:402:NAI:H4N	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:MET:HE2	1:C:58:TYR:CZ	2.46	0.50
1:D:190:PRO:HB2	3:D:403:NAI:H42N	1.96	0.48
1:C:190:PRO:HB2	3:C:402:NAI:H42N	1.97	0.47
1:C:46:PRO:O	1:C:47:GLU:HB3	2.15	0.47
1:D:147:SER:OG	2:D:401:MLI:O8	2.30	0.47
1:D:69:MET:CE	1:D:75:VAL:HG22	2.45	0.47
3:B:402:NAI:O2N	3:B:402:NAI:N7N	2.45	0.45
1:C:146:ALA:O	3:C:402:NAI:H6N	2.16	0.45
1:B:70:LYS:HG2	1:B:118[B]:LEU:HG	1.99	0.45
1:B:98:ILE:HG23	1:B:118[A]:LEU:HD23	1.98	0.44
1:A:110[B]:ASP:OD1	1:A:111:LYS:N	2.51	0.44
1:B:147:SER:OG	2:B:401:MLI:O6	2.33	0.44
1:A:228:ALA:HB3	1:B:251:MET:HE1	1.99	0.44
1:C:32:MET:HE2	1:C:58:TYR:OH	2.18	0.43
1:A:190:PRO:HB2	3:A:402:NAI:H42N	1.99	0.43
1:B:127:THR:HG23	1:B:142:ILE:HD13	1.99	0.43
3:C:402:NAI:H52N	5:C:513:HOH:O	2.18	0.43
2:D:401:MLI:C3	3:D:403:NAI:H4N	2.49	0.43
3:D:403:NAI:C4B	5:D:517:HOH:O	2.65	0.43
3:C:402:NAI:C4B	5:C:513:HOH:O	2.67	0.42
1:D:69:MET:HE3	1:D:75:VAL:HG22	2.00	0.42
1:D:202:ILE:HA	1:D:205:VAL:HG22	2.01	0.42
1:C:70:LYS:HG3	1:C:118:LEU:CD2	2.50	0.41
3:C:402:NAI:O2N	3:C:402:NAI:N7N	2.49	0.41
1:A:22:ILE:HB	3:A:402:NAI:H51N	2.02	0.41
1:A:251:MET:HE1	1:B:228:ALA:CB	2.51	0.41
1:D:16:THR:O	1:D:95:ASN:HB3	2.21	0.41
1:D:7:VAL:HG23	1:D:8:LEU:HG	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/270 (98%)	260 (98%)	4 (2%)	0	100	100
1	B	263/270 (97%)	259 (98%)	4 (2%)	0	100	100
1	C	248/270 (92%)	242 (98%)	6 (2%)	0	100	100
1	D	261/270 (97%)	257 (98%)	4 (2%)	0	100	100
All	All	1036/1080 (96%)	1018 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/206 (98%)	203 (100%)	0	100	100
1	B	201/206 (98%)	201 (100%)	0	100	100
1	C	193/206 (94%)	193 (100%)	0	100	100
1	D	200/206 (97%)	200 (100%)	0	100	100
All	All	797/824 (97%)	797 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	44	GLN
1	C	94	ASN
1	D	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLI	C	401	-	6,6,6	1.58	1 (16%)	7,7,7	1.47	1 (14%)
3	NAI	C	402	-	43,48,48	0.56	0	50,73,73	1.03	4 (8%)
3	NAI	B	402	-	43,48,48	0.54	0	50,73,73	1.01	3 (6%)
4	EDO	D	402	-	3,3,3	0.58	0	2,2,2	0.28	0
3	NAI	A	402	-	43,48,48	0.61	0	50,73,73	1.05	2 (4%)
2	MLI	D	401	-	6,6,6	1.31	1 (16%)	7,7,7	1.62	2 (28%)
2	MLI	B	401	-	6,6,6	1.53	1 (16%)	7,7,7	1.63	2 (28%)
3	NAI	D	403	-	43,48,48	0.60	0	50,73,73	1.11	4 (8%)
2	MLI	A	401	-	6,6,6	1.47	1 (16%)	7,7,7	1.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	C	401	-	-	0/4/4/4	-
3	NAI	C	402	-	-	11/25/72/72	0/5/5/5
3	NAI	B	402	-	-	12/25/72/72	0/5/5/5
4	EDO	D	402	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	A	402	-	-	5/25/72/72	0/5/5/5
2	MLI	D	401	-	-	0/4/4/4	-
2	MLI	B	401	-	-	0/4/4/4	-
3	NAI	D	403	-	-	9/25/72/72	0/5/5/5
2	MLI	A	401	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	MLI	C1-C3	2.58	1.55	1.51
2	B	401	MLI	C1-C3	2.36	1.54	1.51
2	A	401	MLI	C1-C3	2.16	1.54	1.51
2	D	401	MLI	C1-C3	2.12	1.54	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAI	O3D-C3D-C4D	-2.57	103.70	111.08
2	D	401	MLI	O6-C2-C1	-2.52	114.94	122.11
3	C	402	NAI	O3D-C3D-C4D	-2.43	104.11	111.08
3	B	402	NAI	O2D-C2D-C3D	-2.42	104.06	111.82
2	B	401	MLI	O6-C2-C1	-2.41	115.24	122.11
3	B	402	NAI	C5A-C6A-N6A	2.38	123.94	120.31
3	D	403	NAI	O3B-C3B-C4B	-2.36	104.30	111.08
3	D	403	NAI	C5A-C6A-N6A	2.29	123.80	120.31
3	C	402	NAI	O3B-C3B-C4B	-2.29	104.51	111.08
2	C	401	MLI	O6-C2-C1	-2.28	115.62	122.11
2	B	401	MLI	O8-C3-C1	-2.27	115.65	122.11
3	A	402	NAI	C5A-C6A-N6A	2.26	123.76	120.31
3	C	402	NAI	C5A-C6A-N6A	2.26	123.75	120.31
3	D	403	NAI	O2D-C2D-C3D	-2.16	104.88	111.82
3	A	402	NAI	O3D-C3D-C4D	-2.12	104.98	111.08
3	C	402	NAI	O3D-C3D-C2D	-2.09	105.12	111.82
3	D	403	NAI	O3D-C3D-C2D	-2.09	105.12	111.82
2	D	401	MLI	O8-C3-C1	-2.00	116.41	122.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAI	C5D-O5D-PN-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	402	NAI	C5D-O5D-PN-O1N
3	A	402	NAI	C5D-O5D-PN-O2N
3	B	402	NAI	C5B-O5B-PA-O1A
3	B	402	NAI	C5B-O5B-PA-O3
3	B	402	NAI	C5D-O5D-PN-O3
3	B	402	NAI	C5D-O5D-PN-O1N
3	B	402	NAI	C5D-O5D-PN-O2N
3	C	402	NAI	C5B-O5B-PA-O1A
3	C	402	NAI	C5B-O5B-PA-O3
3	C	402	NAI	C5D-O5D-PN-O3
3	C	402	NAI	C5D-O5D-PN-O1N
3	C	402	NAI	C5D-O5D-PN-O2N
3	D	403	NAI	C5D-O5D-PN-O3
3	D	403	NAI	C5D-O5D-PN-O1N
3	D	403	NAI	C5D-O5D-PN-O2N
3	C	402	NAI	C3B-C4B-C5B-O5B
3	C	402	NAI	O4B-C4B-C5B-O5B
3	B	402	NAI	O4B-C4B-C5B-O5B
3	B	402	NAI	C3B-C4B-C5B-O5B
3	D	403	NAI	C3B-C4B-C5B-O5B
3	B	402	NAI	PA-O3-PN-O1N
3	C	402	NAI	PA-O3-PN-O1N
3	A	402	NAI	O4D-C1D-N1N-C6N
3	B	402	NAI	C5B-O5B-PA-O2A
3	C	402	NAI	C5B-O5B-PA-O2A
3	D	403	NAI	O4B-C4B-C5B-O5B
3	A	402	NAI	PA-O3-PN-O1N
3	D	403	NAI	PA-O3-PN-O1N
3	B	402	NAI	O4D-C1D-N1N-C6N
3	D	403	NAI	O4D-C1D-N1N-C6N
3	C	402	NAI	O4D-C1D-N1N-C6N
3	C	402	NAI	C2D-C1D-N1N-C6N
3	B	402	NAI	C2D-C1D-N1N-C6N
3	D	403	NAI	C2D-C1D-N1N-C6N
3	B	402	NAI	PA-O3-PN-O2N
3	D	403	NAI	PA-O3-PN-O2N

There are no ring outliers.

7 monomers are involved in 21 short contacts:

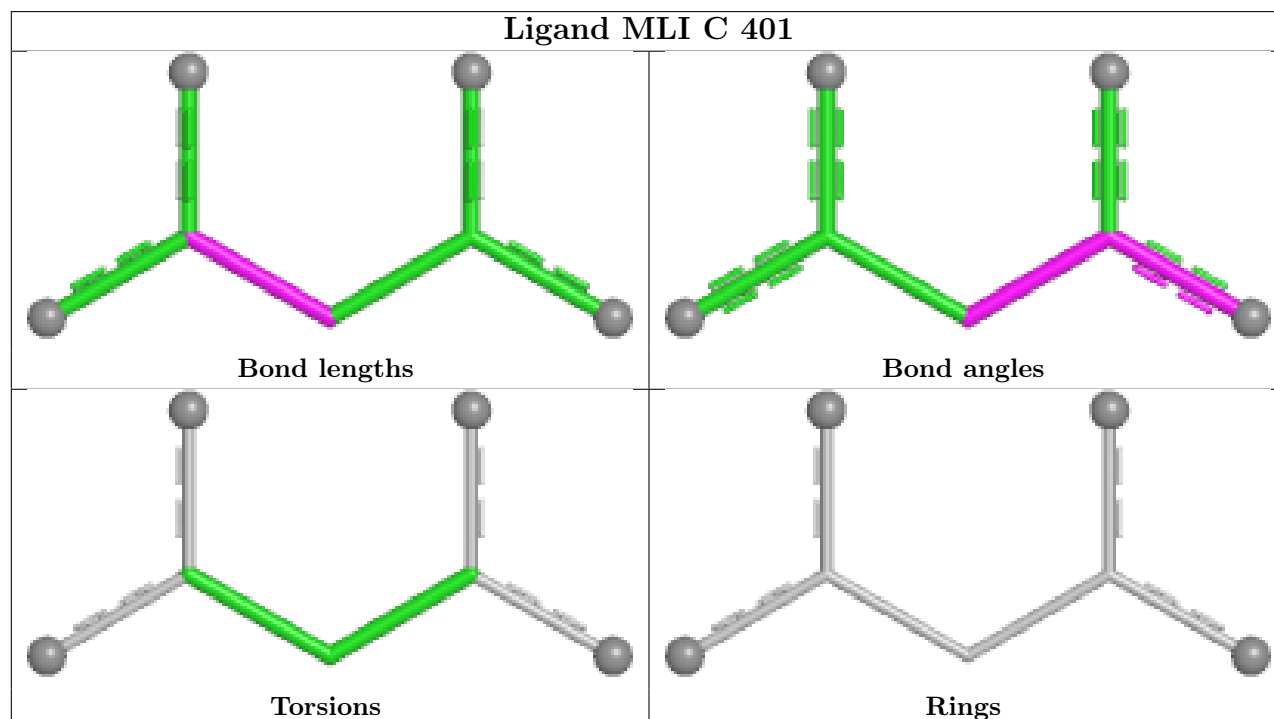
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	MLI	1	0

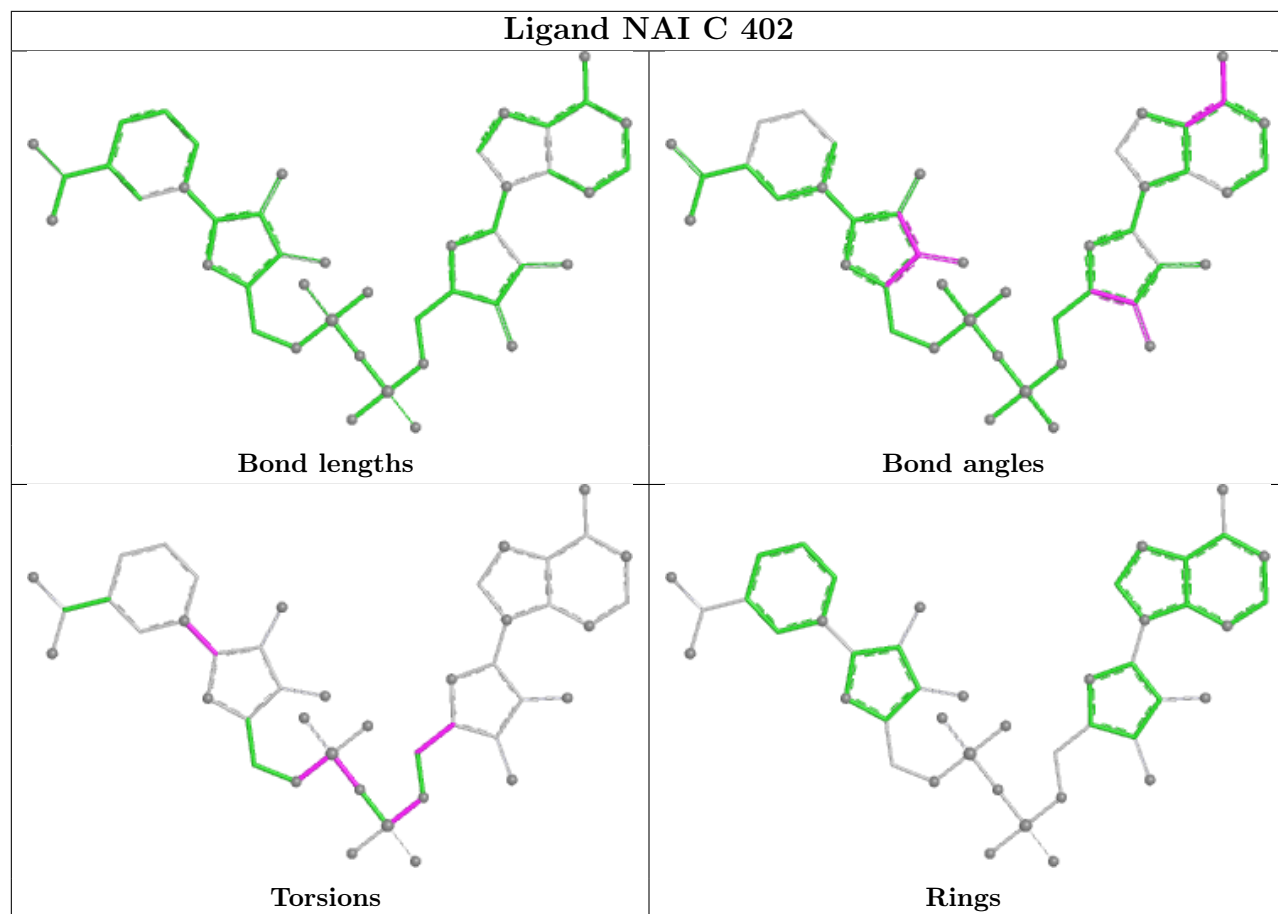
Continued on next page...

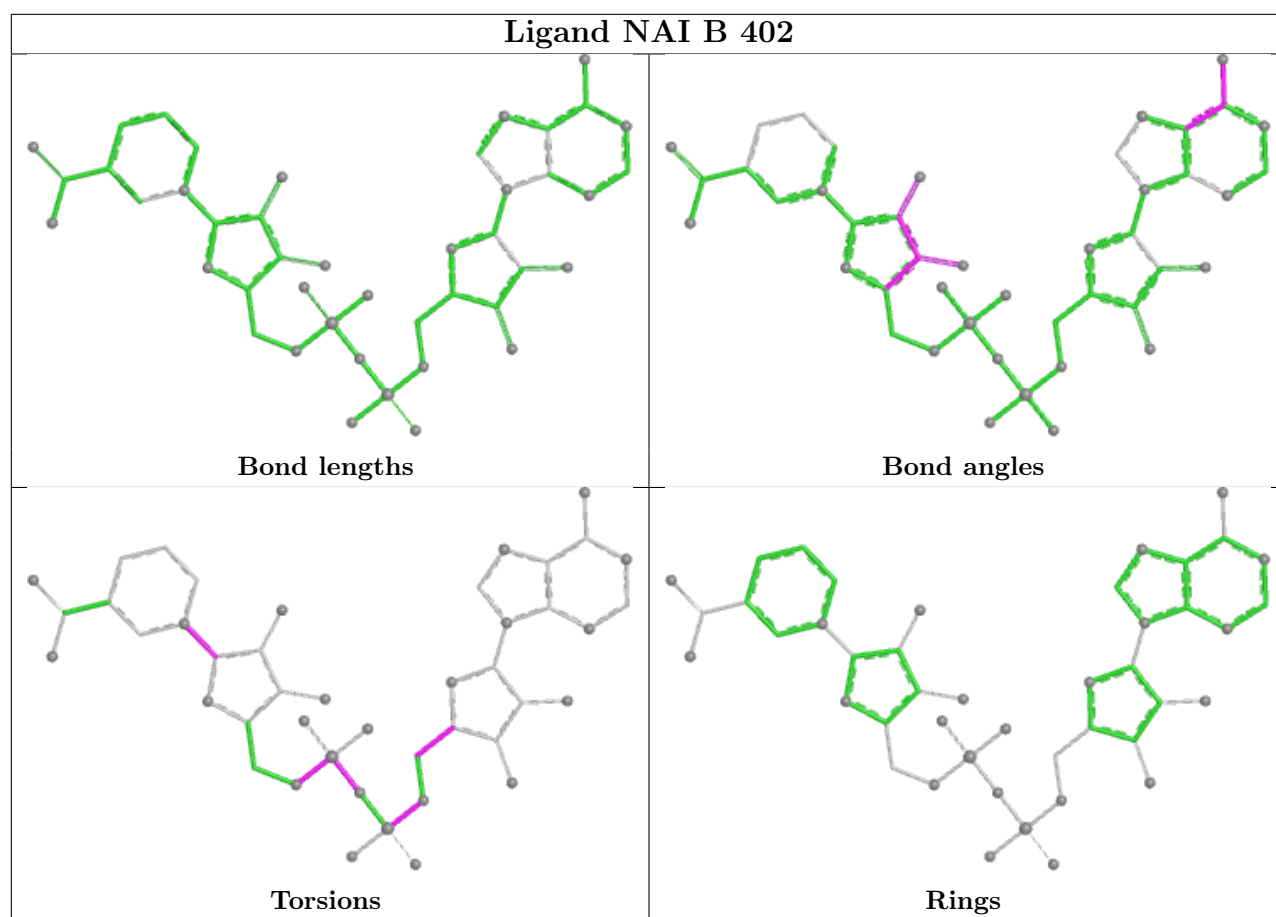
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	NAI	8	0
3	B	402	NAI	4	0
3	A	402	NAI	3	0
2	D	401	MLI	2	0
2	B	401	MLI	2	0
3	D	403	NAI	4	0

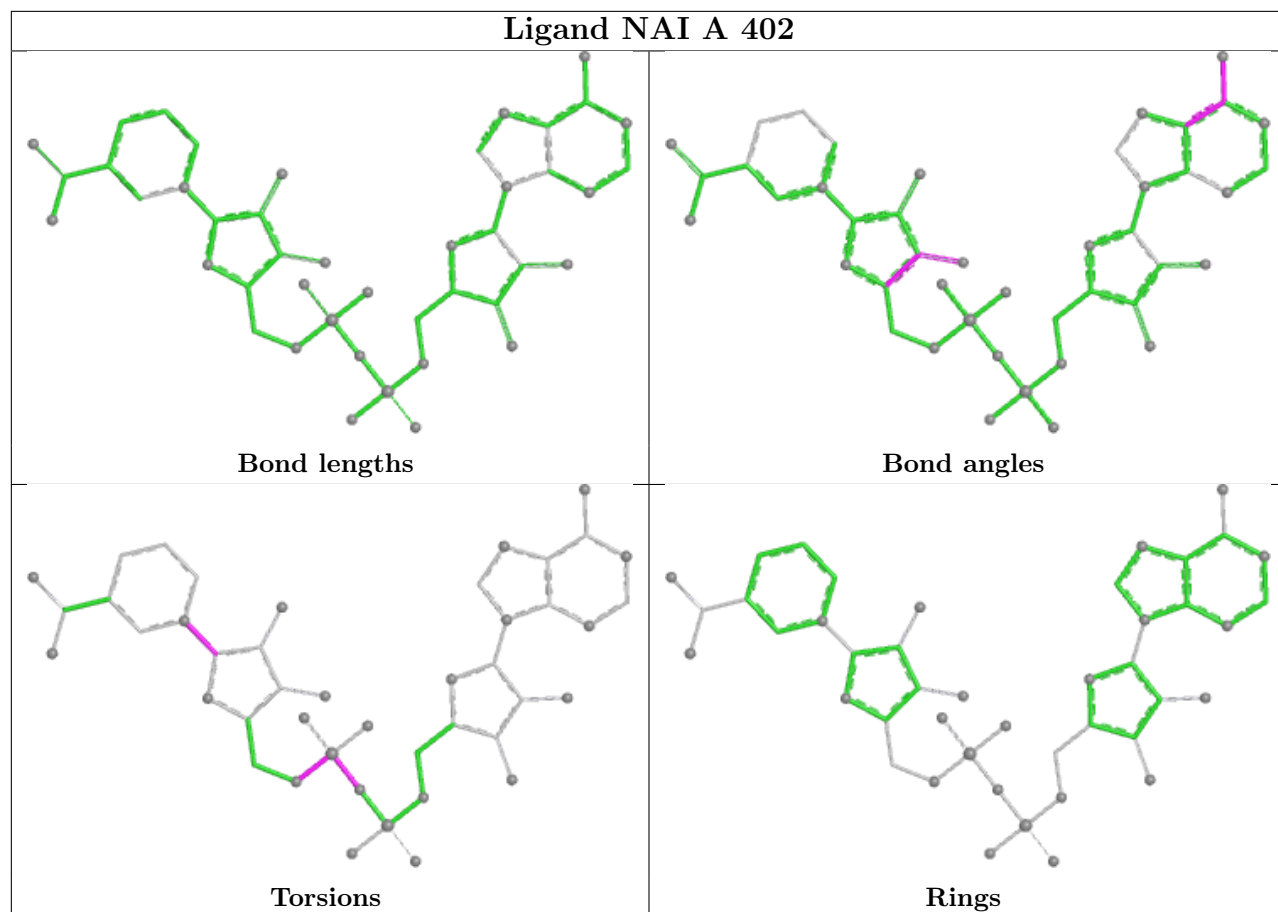
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



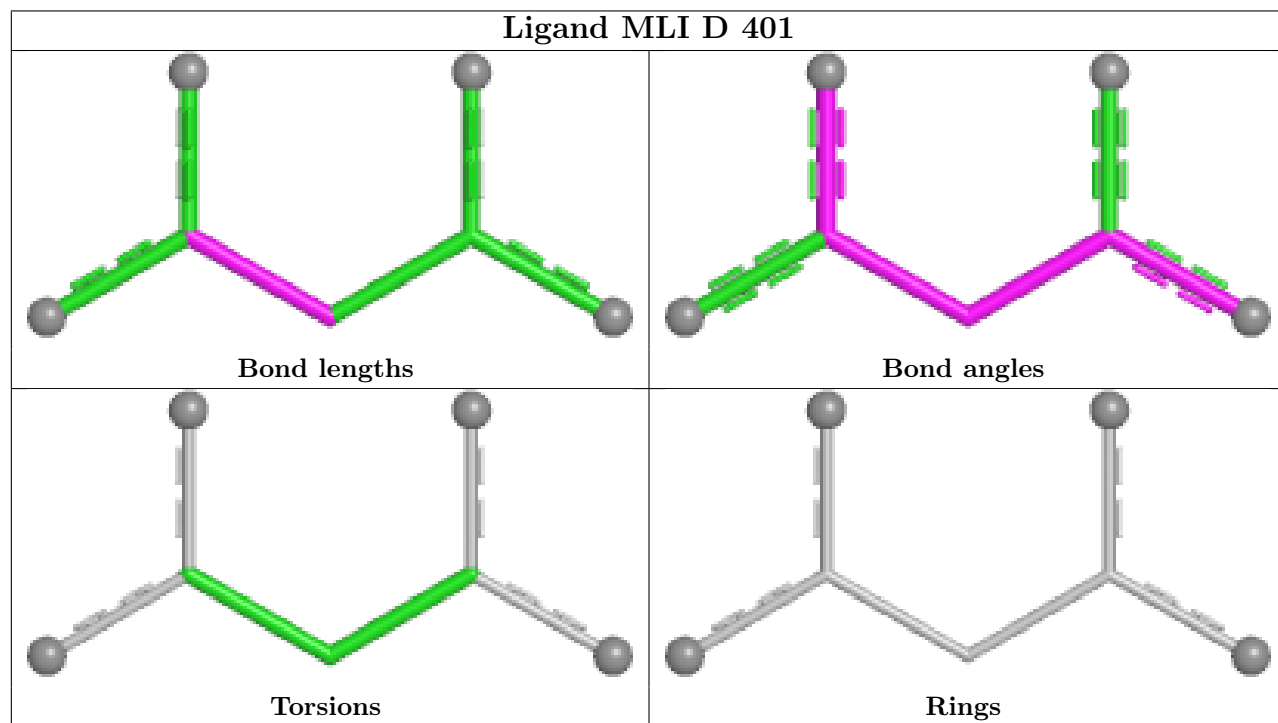


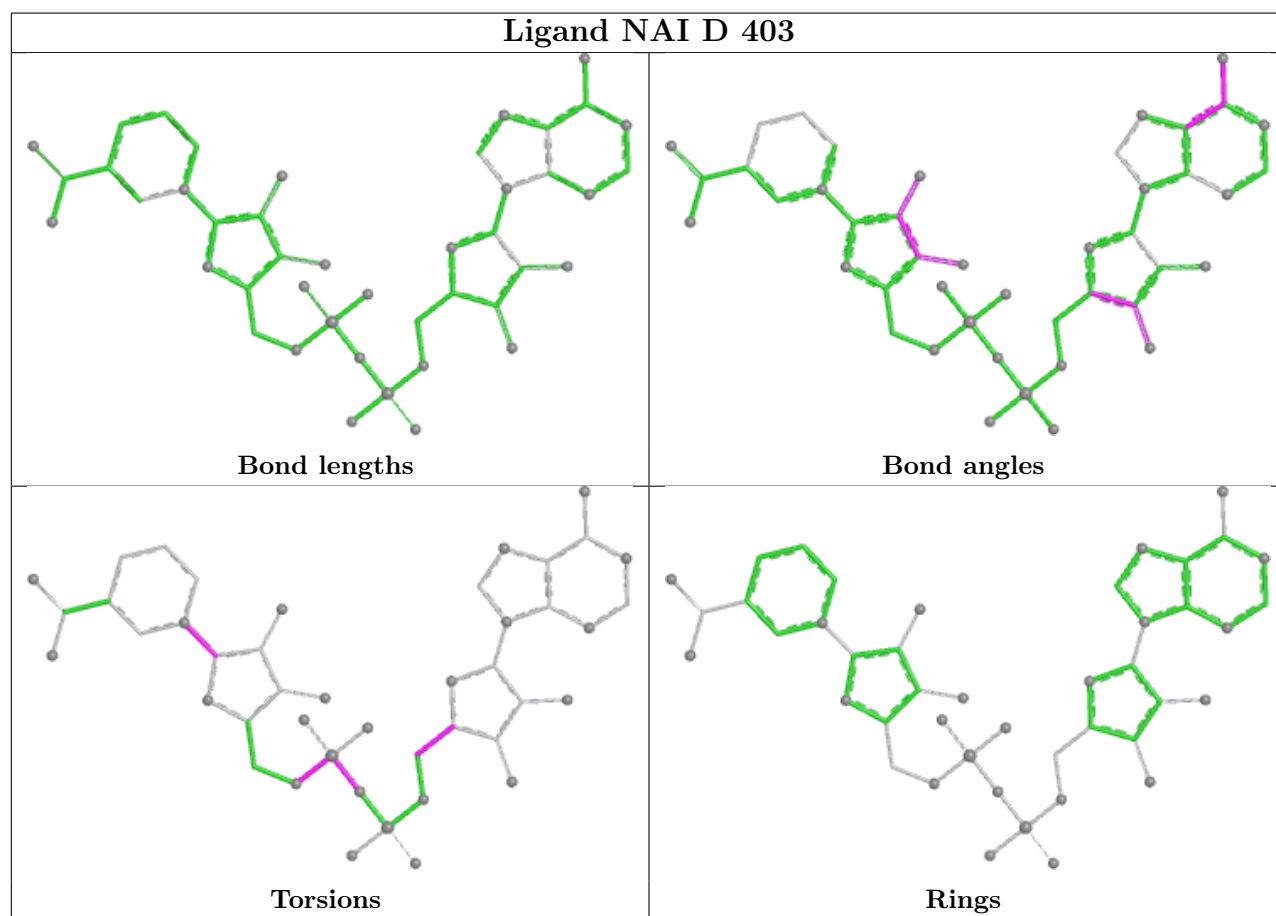
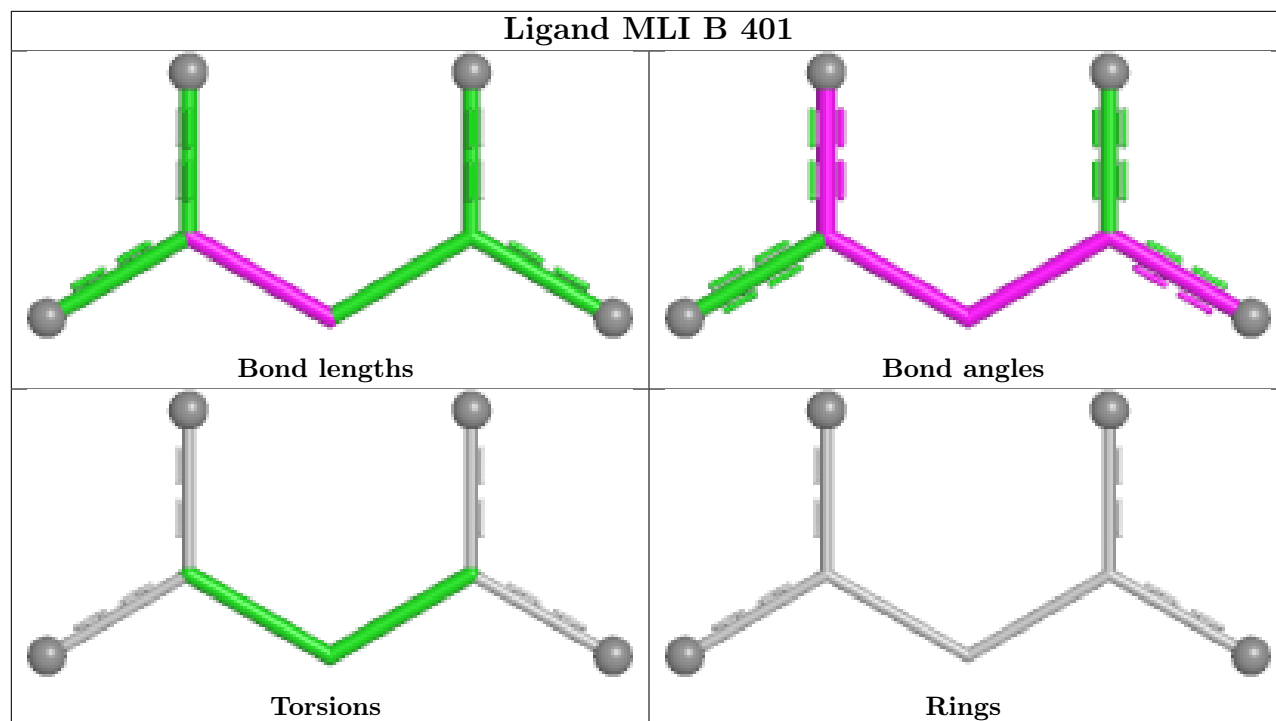


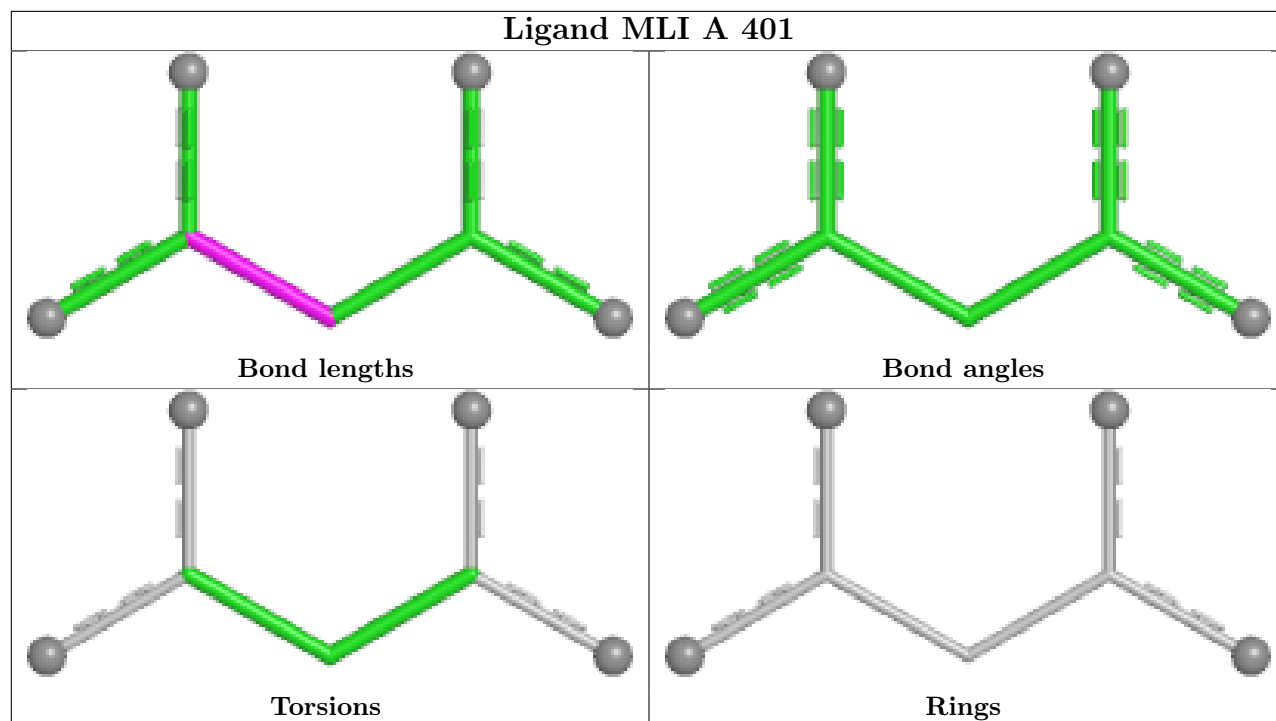
Ligand NAI A 402



Ligand MLI D 401







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/270 (96%)	-0.34	0 100 100	17, 34, 51, 65	3 (1%)
1	B	263/270 (97%)	0.05	19 (7%) 23 22	19, 36, 99, 128	2 (0%)
1	C	247/270 (91%)	-0.14	13 (5%) 33 32	15, 32, 74, 112	5 (2%)
1	D	261/270 (96%)	0.03	5 (1%) 66 68	20, 39, 72, 115	2 (0%)
All	All	1032/1080 (95%)	-0.10	37 (3%) 46 47	15, 35, 72, 128	12 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	7.0
1	C	197	LEU	5.1
1	C	198	VAL	5.1
1	C	96	ALA	4.8
1	D	197	LEU	4.1
1	C	196	PRO	4.0
1	B	216	ALA	3.8
1	C	5	LYS	3.8
1	B	205	VAL	3.7
1	C	46	PRO	3.6
1	B	208	ALA	3.6
1	B	210	TYR	3.4
1	C	217	ALA	3.4
1	B	194	TYR	3.3
1	D	46	PRO	3.2
1	B	198	VAL	3.1
1	B	204	ALA	3.1
1	B	206	ALA	3.0
1	B	213	ASP	3.0
1	C	199	GLU	3.0
1	B	212	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	2.9
1	D	96	ALA	2.6
1	B	196	PRO	2.6
1	B	214	MET	2.5
1	B	223	CYS	2.4
1	D	215	GLU	2.3
1	C	221	PHE	2.3
1	B	211	GLY	2.3
1	C	43	ARG	2.2
1	B	217	ALA	2.2
1	C	47	GLU	2.2
1	B	4	GLU	2.1
1	D	208	ALA	2.1
1	B	219	GLN	2.1
1	C	45	SER	2.0
1	C	118	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLI	B	401	7/7	0.80	0.17	34,38,47,47	9
3	NAI	C	402	44/44	0.80	0.17	31,47,63,76	71
2	MLI	C	401	7/7	0.81	0.18	34,40,48,48	9
3	NAI	B	402	44/44	0.84	0.15	31,47,70,73	71
2	MLI	D	401	7/7	0.88	0.14	32,35,40,40	9
3	NAI	D	403	44/44	0.88	0.13	31,47,71,80	71
2	MLI	A	401	7/7	0.90	0.13	28,31,37,37	9

Continued on next page...

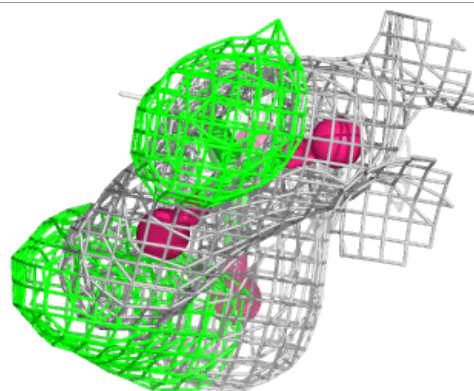
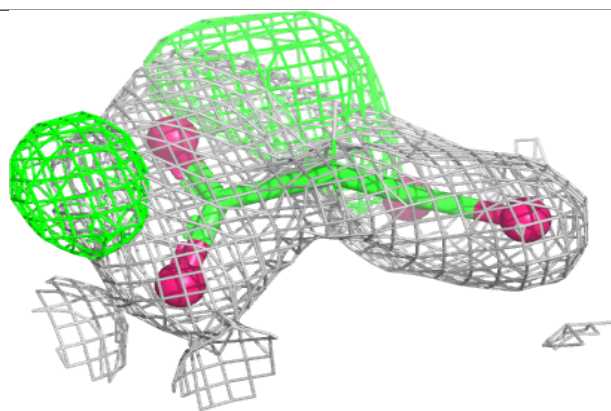
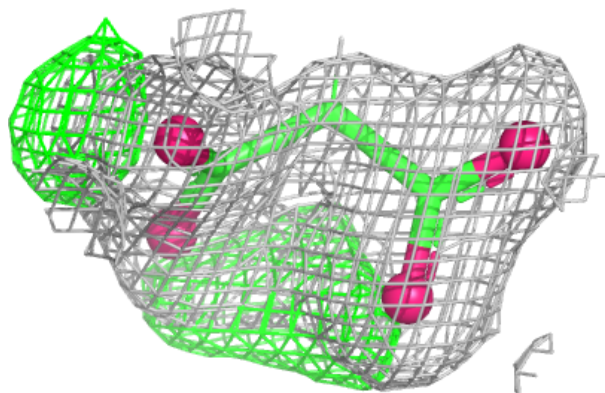
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	D	402	4/4	0.90	0.11	38,45,49,49	0
3	NAI	A	402	44/44	0.93	0.10	25,35,44,47	71

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

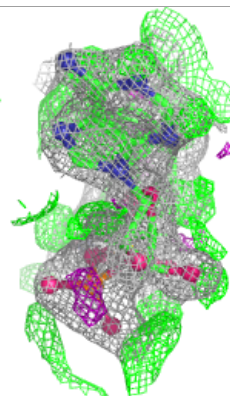
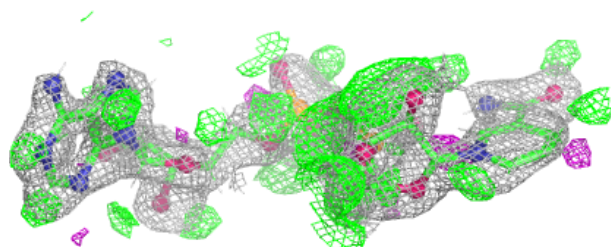
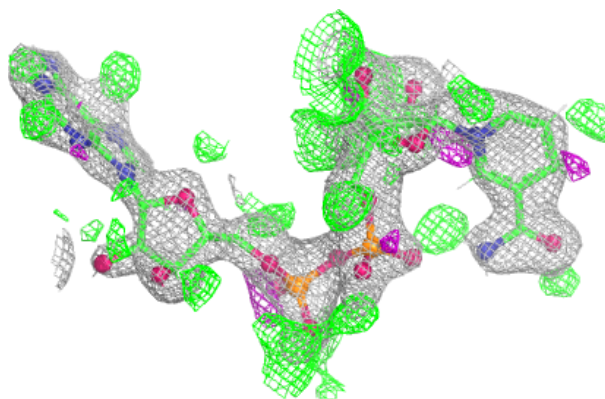
Electron density around MLI B 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

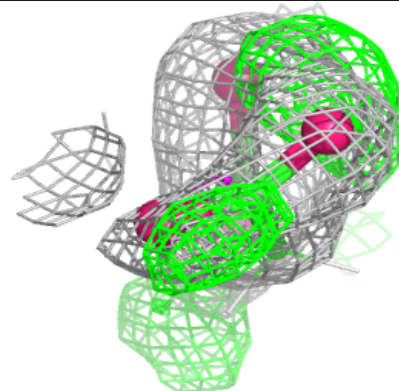
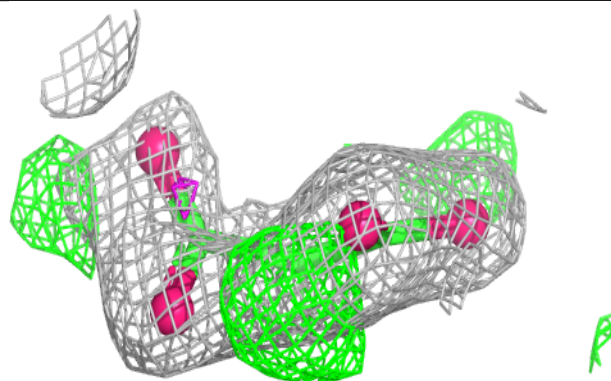
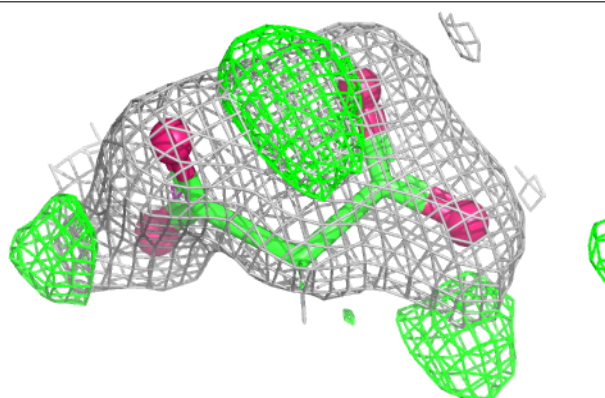


Electron density around NAI C 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

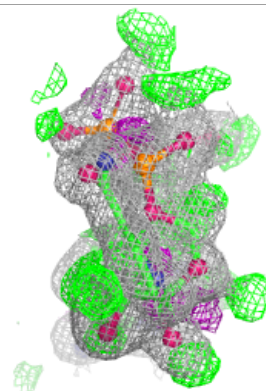
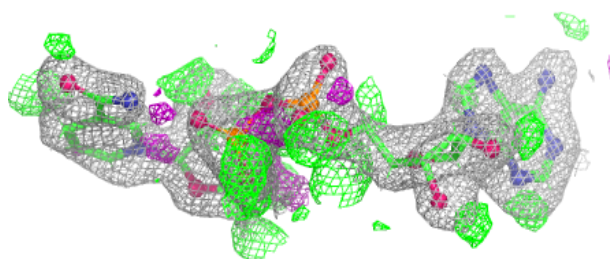
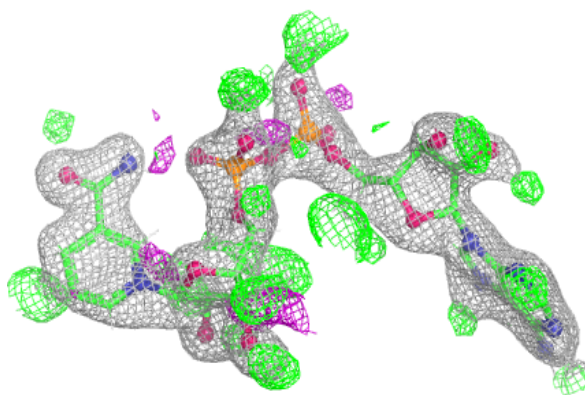
**Electron density around MLI C 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

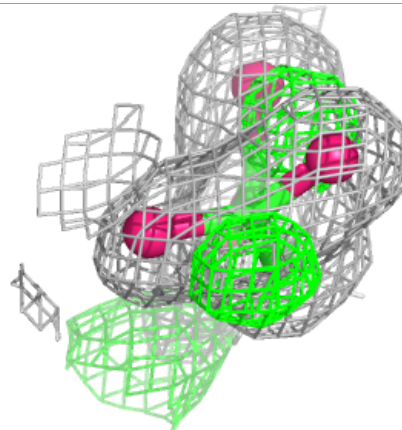
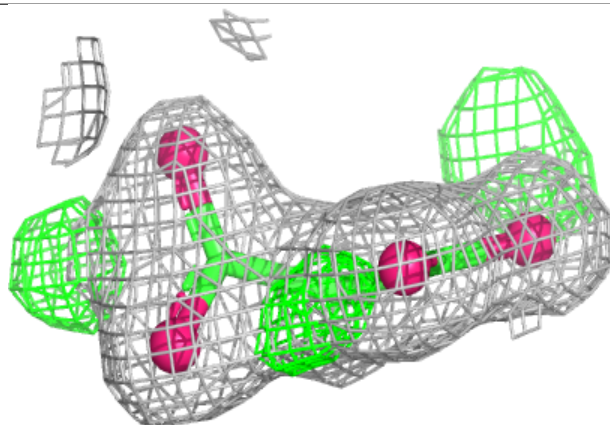
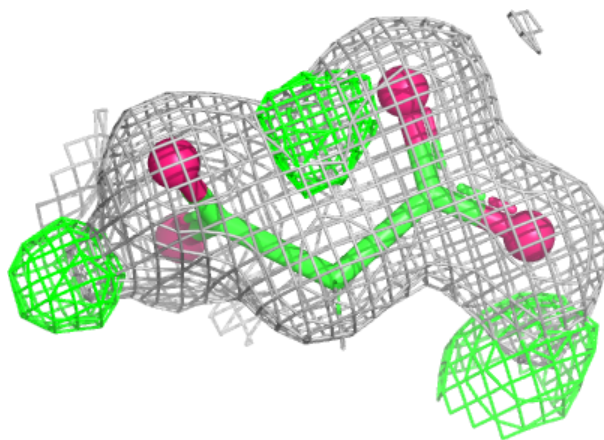


Electron density around NAI B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

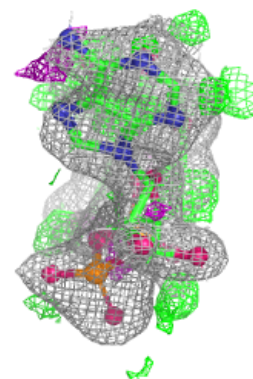
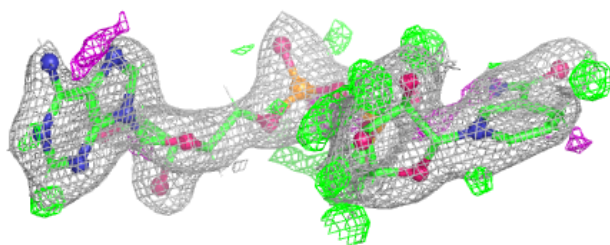
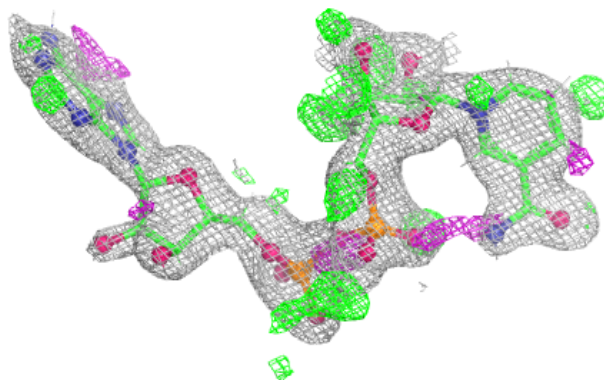
**Electron density around MLI D 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

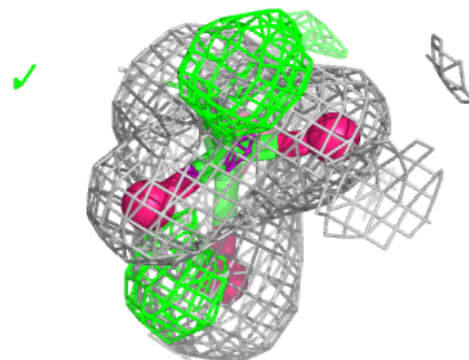
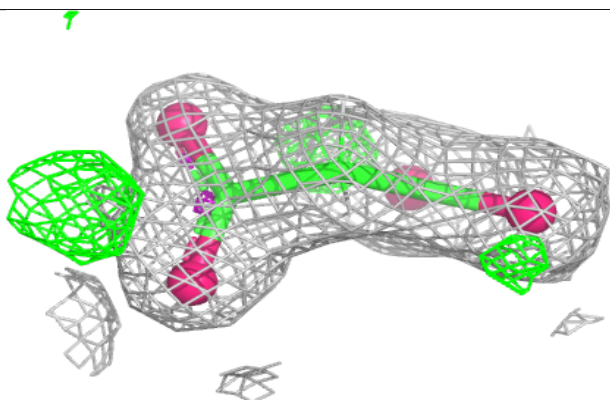
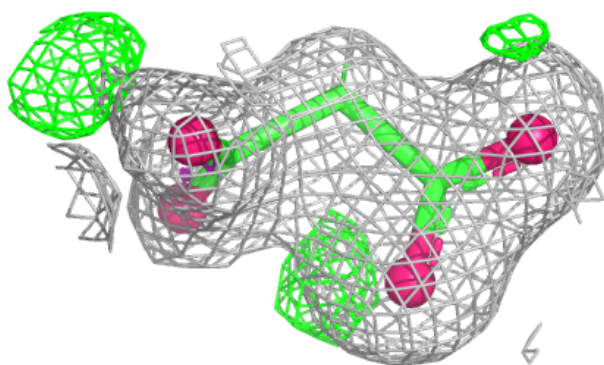


Electron density around NAI D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

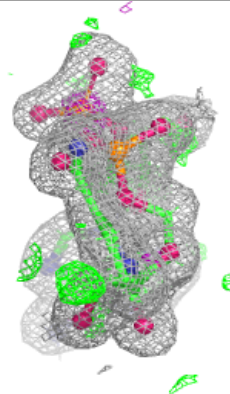
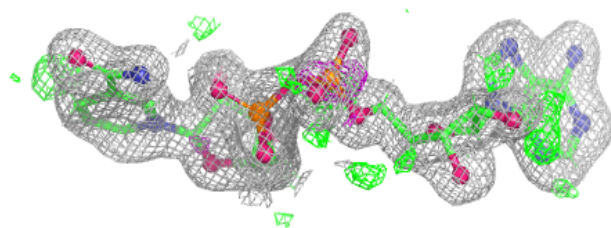
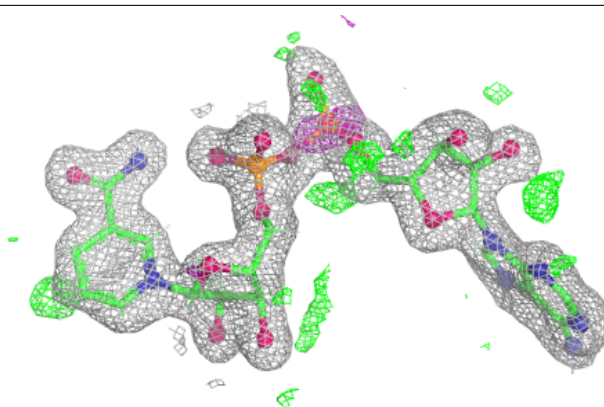
**Electron density around MLI A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAI A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.